

# A microscopic model of ballistic-diffusive crossover

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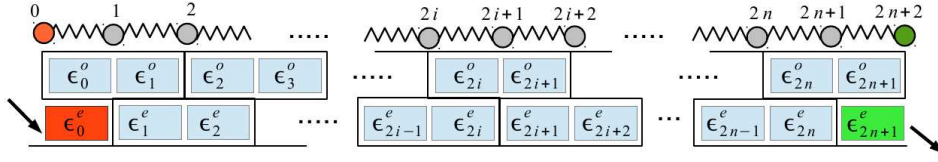
**Abstract.** Several low-dimensional systems show a crossover from diffusive to ballistic heat transport when system size is decreased. Although there is some phenomenological understanding of this crossover phenomena in the coarse grained level, a microscopic picture that consistently describes both the ballistic and the diffusive transport regimes has been lacking. In this work we derive a scaling form for the thermal current in a class of one dimensional systems attached to heat baths at boundaries, and show rigorously that the crossover occurs when the characteristic length scale of the system competes with the system size.

PACS numbers: 66.10.cd, 44.10.+i, 66.70.-f

Low dimensional thermal transport [1, 2, 3] is a field of active research because of its surprises [4, 5] and intriguing features [7, 6]. Most one dimensional (1D) models violate Fourier law and exhibit size dependent thermal conductivity - the examples include harmonic chains [8, 9] the FPU models [10, 11] and the hard point gas model [12, 13, 14]. Some 1D models with unusual scatterers [15, 16], external potential [17, 18, 19] or strong nonlinearity (e. g., interacting classical spins [20, 21]) however obey the Fourier law - the thermal current in 1D scales as  $L^{-1}$  and the thermal conductivity  $\kappa(T)$  is an intensive constant dependent on the temperature and other system parameters. It has been seen that models which show diffusive heat propagation in the thermodynamic limit, also show a crossover to ballistic transport regime when system size is lowered [21, 22, 23]; the crossover scale is usually temperature dependent. This ballistic-diffusive crossover has also been observed experimentally in many low-dimensional systems such as the graphene nanoribbon [6], SiGe nanowires [7], stretched polymer nanofibres [24], carbon nanotubes [25] and other nanowires [26]. Several theoretical attempts have been made [27] to understand this ballistic-diffusive crossover in the coarse grained level, dealing with Boltzmann transport equations [28], scaling theory [21, 29], Langevin dynamics [30], the Buttiker formalism [31] or the nonequilibrium Greens function approach [32] etc. However, a unified microscopic formalism that goes beyond the recent phenomenological attempts [28, 29, 30, 31, 32, 33, 34, 35] and consistently describes both the regimes is still lacking. Here we propose a scaling ansatz for the heat current in driven finite systems in terms of the size and the characteristic length scale of the system. We rigorously derive this scaling form starting from a microscopic dynamics and show that it seamlessly connects the ballistic regime to the diffusive regimes.

Heat transfer in material systems generally involves a wide spectrum of energy carriers, e.g., electrons, phonons, photons, molecules etc., but they operate at different energy and length scales - typically, one of the energy carriers provides the dominant contribution to heat conductivity (see [36] for a comparison of length scales). It is believed that scattering of the carriers, either at the material boundaries or from the impurities, is essential for having normal heat transport. In semiconductors or graphene nano-structures, heat carriers are predominantly phonons which are modeled by the Boltzmann transport equation [23, 28]. As such these studies are not only of theoretical significance but also have immense technological implication [33].

In this article, we formulate a theoretical framework to study this ballistic-diffusive crossover using a few simple 1D models. First we show that the microscopic energy conserving dynamics in these models can be described effectively by classical heat carriers. Next we show that any small scattering probability, either due to collision or interaction with other degrees of freedom, results in diffusive behavior in the thermodynamics limit. Here the thermodynamic limit implies that the system size is much larger than all other characteristic length scales present in the system. The underlying idea of our work is that the characteristic length  $\xi$  of the system (mean free path of the phonons or other carriers, or the spin-spin correlation length in magnetic systems) which is a function of average temperature of the system determines the



**Figure 1.** Spring-mass model with parallel sub-lattice update: Each site of an 1D lattice ( $i = 1, 2, \dots, L = 2n + 1$  for system and  $i = 0, 2n + 2$  for bath) has a particle with position  $x_i$ . The energy is given by Eq. (1). The first (second) row corresponds to the odd (even) site update; boxes in each row depict the neighbouring pair of bond energies  $\epsilon_i^{o,e}$  which are exchanged during the update.

ballistic to diffusive crossover. For  $\xi \gg L$ , the entire system is correlated (mean free path exceeds system size) and the carriers propagate through the system without undergoing scattering and thus we have ballistic transport i.e.  $J \sim L^0$ . In the other case, when  $\xi \ll L$ , the carriers undergo random scattering in the bulk of the system and hence the transport is diffusive  $J \sim L^{-1}$ .

In solid insulators, thermal energy is predominantly transferred by phonons (lattice vibrations); electron movements via collision appear in conductor. We start with a simple 1D model to describe such lattice vibrations classically, which we refer to as the *coupled map lattice model*. Consider a 1D lattice having particles with position variables  $x_i$  ( $i = 1, 2, \dots, L$ ). Let the energy function of the model be defined as

$$E = \frac{k}{2} \sum_{i=1}^L (x_{i+1} - x_i)^2 \quad (1)$$

where  $k$  is the coupling strength and  $L = 2n + 1$  ( $n = 1, 2, \dots$ ). This is similar to the simple harmonic oscillator but without the kinetic energy term.

Using the transformation  $u_i = \sqrt{k/2}(x_{i+1} - x_i)$  Eq. (1) reduces to  $E = \sum_i \epsilon_i$  where  $\epsilon_i = u_i^2$  is the energy of the bond connecting the masses  $i$  and  $i + 1$ . The heat bath is modeled by attaching two masses at the left and right end with coordinates  $x_0$  and  $x_{L+1}$ . These masses oscillate in such a way that the bond energies  $\epsilon_0$  and  $\epsilon_L$  have Boltzmann distribution with temperatures  $\beta_0^{-1}$  and  $\beta_L^{-1}$  respectively, i.e.,

$$P(\epsilon_0) = e^{-\beta_0 \epsilon_0} \quad \text{and} \quad P(\epsilon_L) = e^{-\beta_L \epsilon_L}. \quad (2)$$

To study energy transport in this model we use a local odd-even parallel update scheme, where lattice sites belonging to the even and odd sublattice are updated synchronously. To mimic the equation of motion, which conserves the total energy, we implement a dynamical rule so that the energy is conserved locally. When a site  $i$  is updated without disturbing the neighbors  $i \pm 1$  (which belong to a different sublattice), both  $u_i$  and  $u_{i+1}$  are updated keeping their sum  $u_i + u_{i+1} = x_{i+1} - x_{i-1}$  unaltered. Along with this constraint, energy conservation also demands that  $u_i^2 + u_{i+1}^2$  must be conserved. Thus the only possible solutions are

$$(u_i \rightarrow u_i, u_{i+1} \rightarrow u_{i+1}) \quad \text{or} \quad (u_i \rightarrow u_{i+1}, u_{i+1} \rightarrow u_i).$$

Clearly, the first solution does not update the positions  $\{x_i\}$  and we chose to work with the second which effectively exchanges the energies  $\epsilon_i$  and  $\epsilon_{i+1}$  of the bonds connected to the  $i$ -th site. As can be seen from Fig. 1, during the odd sublattice update, the energies  $\epsilon_i^o$ , of the bond that connect mass  $i$  and  $i + 1$ , are exchanged pairwise:  $\epsilon_0^o \rightleftharpoons \epsilon_1^o, \epsilon_2^o \rightleftharpoons \epsilon_3^o, \dots, \epsilon_{2n}^o \rightleftharpoons \epsilon_{2n+1}^o$ . For the even sublattice update, energy exchange similarly occurs between  $\epsilon_1^e \rightleftharpoons \epsilon_2^e, \dots, \epsilon_{2n-1}^e \rightleftharpoons \epsilon_{2n}^e$  and the boundary energies  $\epsilon_0^e$  and  $\epsilon_L^e$  are refreshed by random values drawn respectively from the Boltzmann distributions Eq. (2). Effectively, the energy which is introduced to the system at the site  $i = 0$  ( $i = L$ ) moves one step to the right (left) during each sublattice update and goes out of the system through the other end exactly after  $L$  odd-even updates. This undeflected motion of the energy packets would result in ballistic heat-transport. In the stationary state we have

$$\langle \epsilon_{2i}^o \rangle = \langle \epsilon_L \rangle ; \langle \epsilon_{2i+1}^o \rangle = \langle \epsilon_0 \rangle ; \langle \epsilon_{2i}^e \rangle = \langle \epsilon_0 \rangle ; \langle \epsilon_{2i+1}^e \rangle = \langle \epsilon_L \rangle. \quad (3)$$

and thus the energy current  $J = \langle \epsilon_{2i}^e \rangle - \langle \epsilon_{2i}^o \rangle$  is independent of the system size. This result is same as the ballistic transport observed in the simple harmonic lattice [8] with usual Hamiltonian dynamics, the only difference being the absence of the kinetic term here.

*Scattering of heat carriers:* In order to have normal transport we need to introduce some scattering mechanism in this model, which can change right movers (generated at the left end of the system) to left movers and vice versa. This can be incorporated if, during an update, particles change their position  $x_i$  with a nonzero probability  $p$ , i.e., now both the solutions of Eq. (3) are chosen (the first one with probability  $1 - p$  or otherwise the second one). Thus,

$$(\epsilon_i, \epsilon_{i+1}) \xrightarrow{1-p} (\epsilon_i, \epsilon_{i+1}); \quad (\epsilon_i, \epsilon_{i+1}) \xrightarrow{p} (\epsilon_{i+1}, \epsilon_i). \quad (4)$$

This modified dynamics produces a scattering of both right and left movers with probability  $q = 1 - p$ . Thus the stationary energy profile must satisfy the following equations.

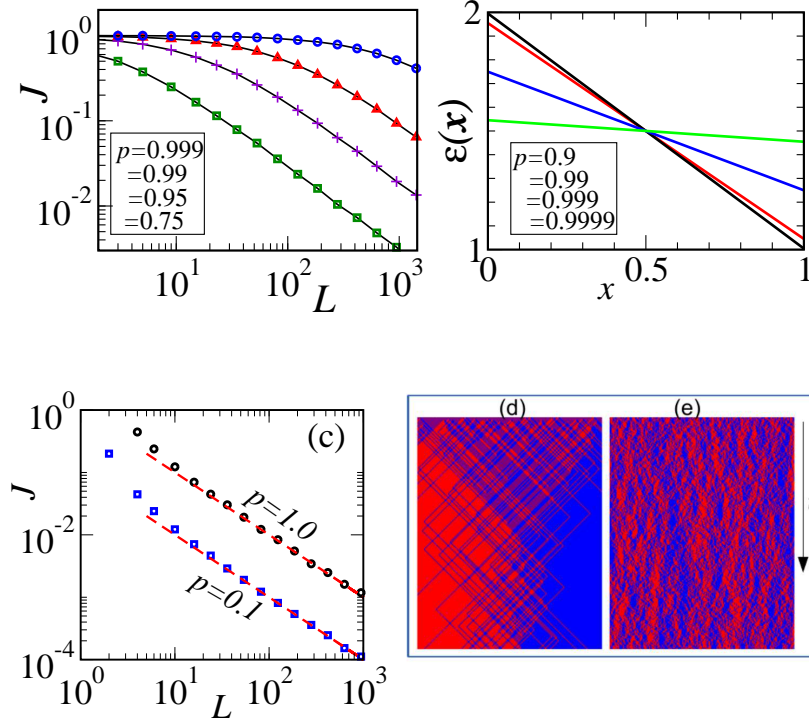
$$\begin{aligned} \epsilon_{2i}^o &= q\epsilon_{2i}^e + p\epsilon_{2i+1}^e ; \quad \epsilon_{2i+1}^o = q\epsilon_{2i+1}^e + p\epsilon_{2i}^e; \\ \epsilon_{2i}^e &= q\epsilon_{2i}^o + p\epsilon_{2i-1}^o ; \quad \epsilon_{2i-1}^e = q\epsilon_{2i-1}^o + p\epsilon_{2i}^o, \end{aligned} \quad (5)$$

where  $\epsilon_i^{o,e}$  are the average energy of the bond energy after odd and even sublattice updates. In the second equation, which stands for even sublattice update,  $i$  runs from 1 to  $n - 1$  and the boundary energies must satisfy  $\epsilon_0^e = \langle \epsilon_0^e \rangle$ ,  $\epsilon_{2n+1}^e = \langle \epsilon_L^e \rangle$ . This set of equations can be solved along with the boundary conditions, resulting in

$$\begin{aligned} \epsilon_{2i}^e &= (1 - 2iq)\epsilon_0^e + 2iq\epsilon_1^e \\ \epsilon_{2i+1}^e &= -2iq\epsilon_0^e + (1 + 2iq)\epsilon_1^e. \end{aligned} \quad (6)$$

Thus the steady state energy profile  $\langle \epsilon_i \rangle = \frac{1}{2}(\langle \epsilon_i^e \rangle + \langle \epsilon_i^o \rangle)$  can be written, taking  $x = i/L$  and  $\Delta E = \langle \epsilon_0 \rangle - \langle \epsilon_L \rangle$ , as

$$\epsilon(x) = \langle \epsilon_0 \rangle + \frac{p\Delta E}{2(Lq + p)} - \frac{\Delta E}{(1 + p/Lq)}x. \quad (7)$$



**Figure 2.** (a) Energy current  $J$  versus  $L$  (simulation results (symbols) are compared with Eq. (8) in solid line, and (b) the energy profile  $\epsilon(x)$  for different  $p$ . Here  $\langle\epsilon_0\rangle = 2$ ,  $\langle\epsilon_L\rangle = 1$  and ballistic limit is approached when  $p \rightarrow 1$ . (c)  $J$  versus  $L$  for the model with random-sequential dynamics which results in diffusive transport even when  $p = 1$ . (d) and (e) show evolution of the system for odd-even parallel and random-sequential dynamics respectively with  $p = 0.95$  and  $L = 200$ . Energy carriers introduced at the hot (left) and cold (right) boundaries are marked with different colors (red and blue).

Here  $L = 2n + 1$  is system size (excluding the two sites  $i = 0, L$  which are considered to be part of the heat reservoir). Clearly the profile is linear, but there are boundary layers at both ends (second term in above equation) which vanish when  $L \rightarrow \infty$ . For any finite  $L$ , however, the profile becomes flat when  $p \rightarrow 1$  (see Fig. 2(b)) - an indication that energy transport occurs ballistically in this limit. Now the thermal current (Fig. 2(a)) is

$$J = \epsilon_0^e - \epsilon_0^o = p(\epsilon_0^e - \epsilon_1^e) = p \frac{\Delta E}{Lq + p}. \quad (8)$$

Thus, for any  $p < 1$ , the coupled map lattice model shows diffusive transport with conductivity  $\kappa = p/q$  and is independent of system size. The deterministic limit  $p = 1$  however shows ballistic transport with heat current being independent of the system size. Thus, diffusive behaviour here is a consequence of stochasticity which provides a scattering mechanism for the heat carriers, even though energy is conserved. In fact if stochasticity is introduced differently, say by using a random sequential dynamics in this model instead of parallel sublattice update, we get diffusive transport even for  $p = 1$  (see Fig. 2(c)). To get a more physical picture of this ballistic-diffusive crossover let us

rewrite  $J$  as

$$J = \kappa \frac{\Delta E}{L} \mathcal{F}\left(\frac{\xi}{L}\right) \quad (9)$$

where  $\xi = 1/q$  is the relevant length scale (see discussions below) and  $\mathcal{F}(x)$  is the scaling function. In general  $\mathcal{F}(x)$  has the following property:  $\mathcal{F}(0) = 1$  and  $\mathcal{F}(x) \sim 1/x$  for large  $x$  and for this simple model,  $\mathcal{F}(x) = \frac{1}{1+px}$ . In fact, this scaling form is not accidental, we argue that such a scaling form always occurs in models of heat conduction and becomes prominent only near the ballistic limit, where the dominant length scale of the system  $\xi$  competes with the system size  $L$ . This situation may arise near a critical point (where  $\xi$  is the correlation length), in low dimensional disordered systems ( $\xi$  is the localization length), and in colliding particle systems ( $\xi$  is the mean-free path).

The model discussed here, can be interpreted as though energy carriers (say phonons) are generated randomly and independently at both boundaries. At the left (right) end they are generated with unit rate as right (left) movers to carry an energy unit  $\epsilon_0(\epsilon_L)$  drawn from a Boltzmann distribution; they move in assigned directions (left or right) synchronously with unit rate and may change their direction with probability  $q$  (see Fig. 2(d) for evolution of the left and right movers). Thus they can move exactly  $n$  steps persistently with probability  $qe^{-n/\xi}$  where  $\xi = |\ln p|^{-1}$  is the persistent length which diverges in the limit  $q \rightarrow 0$ . In this limit  $\xi = |\ln(1 - q)|^{-1} \sim q^{-1}$ .

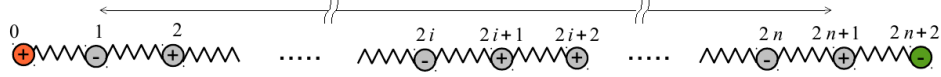
In a recent work [22] a model of persistent walkers has been studied on a 1D lattice with asynchronous (continuous time) update rules, where the right and left moving walkers can get interchanged at a small rate  $p$ . These persistent walkers keep moving along one direction until they convert to the other type, generating a characteristic length scale similar to the mean free path of free carriers in a solid. This gives rise to a length scale in the system. The authors showed that the electrical current can be expressed as

$$J_{el} = \frac{\ell v \Delta \rho}{L(1 + \ell/L)} \quad (10)$$

where  $\ell$  is the coherence length scale,  $v$  being the mean velocity and  $\Delta \rho$  the difference in carrier density of left and right reservoirs. Comparing this result with Eq. (8), we find that in our model  $\ell \equiv p/q$  and  $v = 1$  here. From purely phenomenological arguments, an expression similar to Eqs. (8), (10) energy transmission in carbon nanotubes [32, 31], current in Heisenberg model [21] has been introduced recently; a more generic scaling form, Eq. (9), has also been obtained for conductivity in anharmonic chains [29].

*Spring mass-spin model:* Until now we have discussed models where heat carriers move independently. It is important to know if Eq. (9) still holds for a system in which the motion of heat carriers is correlated. To this end, we introduce the following model. Let us assume that every particle  $i$  of the spring mass model has a spin  $s_i = \pm$ . These Ising spins interact ferromagnetically, as described in Fig. 3 and evolve following the Glauber dynamics

$$\pm \xrightarrow{1-\Delta V} \mp, \quad \text{where } V = -\frac{K}{4} \sum_{i=0}^L s_i s_{i+1} - h s_0. \quad (11)$$



**Figure 3.** Spring mass-spin model: Particle at each site  $i$  of the lattice ( $i = 1, 2, \dots, L = 2n + 1$  for system and  $i = 0, 2n + 2$  for bath) has a spin  $s_i = \pm$ , along with the position variable  $x_i$ , which evolve following Eq. (11).

The magnetic field  $h$  at the left boundary controls the magnetization profile of the system. The masses follow the parallel sublattice update rule with the energy function given by Eq. (11), but now  $x_i$  is updated (i.e., associated bond energies  $\epsilon_i$  and  $\epsilon_{i+1}$  are exchanged) only when  $s_i = +$ . In this simple model, the spatial spin-spin correlation affects the energy transport even though the spins do not take part directly and dictate only the update dynamics of the particles.

For simplicity, let us consider  $h \rightarrow \infty$  limit, which forces the spin at site  $i = 0$  to be  $s_0 = +$ . The stationary probability  $p_i$  that  $s_i = +$  at site  $i$ , can be calculated from the standard transfer matrix  $\langle s|T|s' \rangle = \exp(Kss'/4)$  as

$$p_i = \frac{1}{2} [1 + \tanh^i(K/4)] . \quad (12)$$

Now,  $p_i$  is the scattering probability of the heat carriers at the lattice site  $i$ . In other words,  $p_i$  is the probability that a left (right) moving energy carrier becomes a right (left) mover at site  $i$ .

We proceed with a generic function  $p_i$ , and will finally consider Eq. (12) as a special case. Following the steps similar to the  $p_i = p$  case, we find that in steady state, the average energies after odd-sublattice update are

$$\epsilon_{2i}^o = q_{2i+1}\epsilon_{2i}^e + p_{2i+1}\epsilon_{2i+1}^e; \quad \epsilon_{2i+1}^o = q_{2i+1}\epsilon_{2i+1}^e + p_{2i+1}\epsilon_{2i}^e,$$

and the same after even-sublattice update ( $i = 1, 2, \dots, n - 1$ ) are

$$\epsilon_{2i}^e = q_{2i}\epsilon_{2i}^o + p_{2i}\epsilon_{2i-1}^o; \quad \epsilon_{2i-1}^e = q_{2i}\epsilon_{2i-1}^o + p_{2i}\epsilon_{2i}^o,$$

where  $q_i = 1 - p_i$ . These equations need to be solved with boundary conditions  $\epsilon_0^e = \langle \epsilon_0 \rangle$  and  $\epsilon_L^e = \langle \epsilon_L \rangle$ . It is now straightforward to obtain the energy profile (after odd-sublattice update),

$$\begin{aligned} \epsilon_{2i}^e &= (1 - \lambda_i)\langle \epsilon_0 \rangle + \lambda_i\epsilon_1^e, \quad \epsilon_{2i+1}^e = \epsilon_{2i}^e + p_1 \frac{\langle \epsilon_0 \rangle - \epsilon_1^e}{p_{2i+1}} \\ &\text{with } \lambda_i = p_1 \sum_{j=1}^{2i+1} p_j^{-1} - 2p_1 i. \end{aligned} \quad (13)$$

To calculate the energy profile explicitly we need  $\epsilon_1^e$ ; the boundary condition  $\epsilon_{2n+1}^e = \langle \epsilon_L \rangle$  gives

$$\epsilon_1^e = \frac{(\lambda_n - 1)\langle \epsilon_0 \rangle + \langle \epsilon_L \rangle}{\lambda_n} = \langle \epsilon_0 \rangle - \frac{\Delta E}{\lambda_n}. \quad (14)$$

It is evident, from Eqs. (8) and (14), that the energy current is

$$J = p_1 \frac{\Delta E}{\lambda_n} \simeq \frac{\Delta E}{L(\alpha_1 - 1) + 1} \quad (15)$$



where in the last step we have taken the continuum limit  $x = i/L$  to write Eq. (13) as,

$$\lambda_n \simeq p_1[L(\alpha_1 - 1) + 1] \quad \text{with} \quad \frac{d\alpha_x}{dx} = \frac{1}{p(x)} \quad (16)$$

In the continuum limit, the energy profile (from (13)) is

$$\epsilon(x) = \epsilon_0 + \frac{\Delta E}{2L(\alpha_1 - 1) + 1} - \Delta E \frac{L(\alpha_x - 1) + 1}{L(\alpha_1 - 1) + 1}.$$

Note, that for a given boundary drive, both current and energy profile depend *only on* the scattering probability  $p(x)$  (through  $\alpha_x$  from Eq. (16)); details of the dynamics, interaction or disorder plays a role in generating a spatial variation of scattering. These exact results, though derived here for a class of interacting systems driven at boundaries, are expected to be generic; it explains in general, why current and density profile in driven systems depend only on the scattering probability of the current-carriers in the bulk of the sample.

Evidently the current  $J$  in Eq. (15) becomes ballistic when  $\alpha_1 = 1$  and for any  $\alpha_1 > 1$  one gets the Fourier law in the thermodynamic limit  $L \gg (\alpha_1 - 1)^{-1}$ . Thus  $(\alpha_1 - 1)^{-1}$  plays the role of correlation length  $\xi$ , which diverges in the limit  $\alpha_1 \rightarrow 1$ . To verify that  $(\alpha_1 - 1)$  actually plays the role of  $\xi^{-1}$ , let us consider a simple example  $p(x) = e^{-\gamma x}$  where  $\gamma^{-1}$  is a measure of spatial correlation. Now  $\alpha_1 - 1 = \gamma^{-1}(e^\gamma - 1 - \gamma)$  which, for small  $\gamma$ , gives  $\gamma/2$ . Thus  $J = \Delta E/(1 + L\gamma/2)$  is consistent with the ansatz (9). Again, for a spring mass-spin model  $p_i$  is given by Eq. (12); then  $\alpha_1 - 1 \simeq |\ln(\tanh(K/4))|/4$ , which is inversely proportional to the correlation length known for Ising model. Also note that for  $p_i = p$  we trivially recover the result Eq. (8) from Eq. (15).

*Discussion:* The model that we have introduced here can be considered to be formally identical to a system of free particles with momentum  $p_i$ ,  $H = \sum_i p_i^2/2m$ . The odd-even dynamics is nothing but the integration of the equation of motion using a finite integration time step  $\Delta t$ . The additional constraint introduced in spring mass system, i.e.,  $u_i + u_{i+1}$  is not altered during update of  $x_i$ , translates to momentum conservation during collision of particles  $i$  and  $i + 1$ . Finally, the scattering probability  $p$  in spring mass system becomes the collision probability. Thus one obtains ballistic transport when collision occurs pairwise and deterministically, whereas energy transport is diffusive when collisions are missed out with finite probability. Using these simple models we have proven rigorously that the scaling ansatz proposed for the current, Eq. (9) can seamlessly describe both the ballistic transport regime with the diffusive regime. There are however a few drawbacks of the current formalism. Firstly, the heat carriers are assumed to carry a quantized packet of energy with them which does not get scattered and redistributed, and therefore unrealistic for real life transport problems. Secondly in the spring mass-spin model, introduced as a model with spatial correlation, the dynamics of the background spins is completely decoupled from that of the heat carriers. It remains a challenge to address these issues in the future.

*Acknowledgments:* PKM would like to acknowledge the support of CEFIPRA under Project 4604-3.



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